

Fig. 1

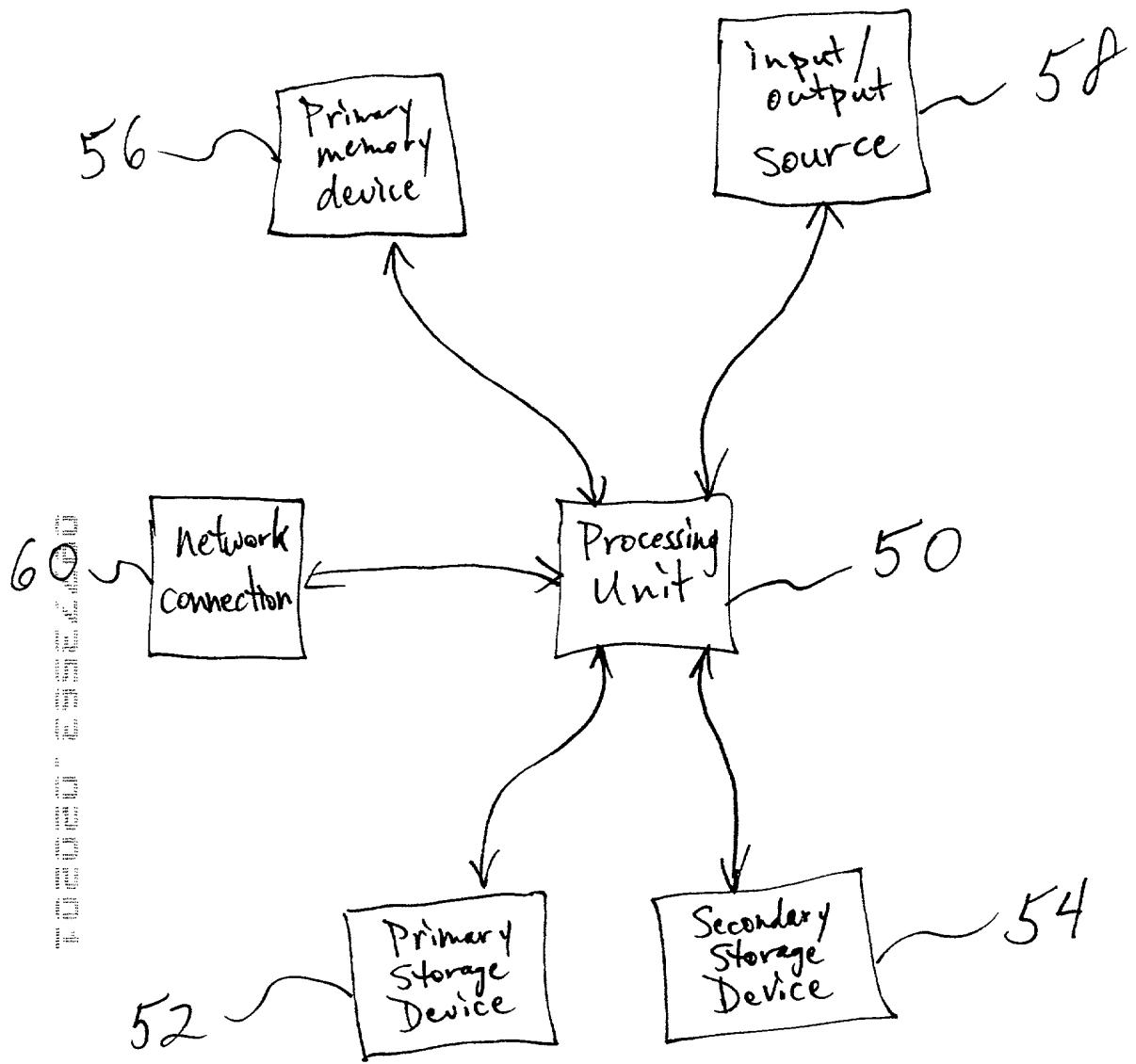


Fig. 2

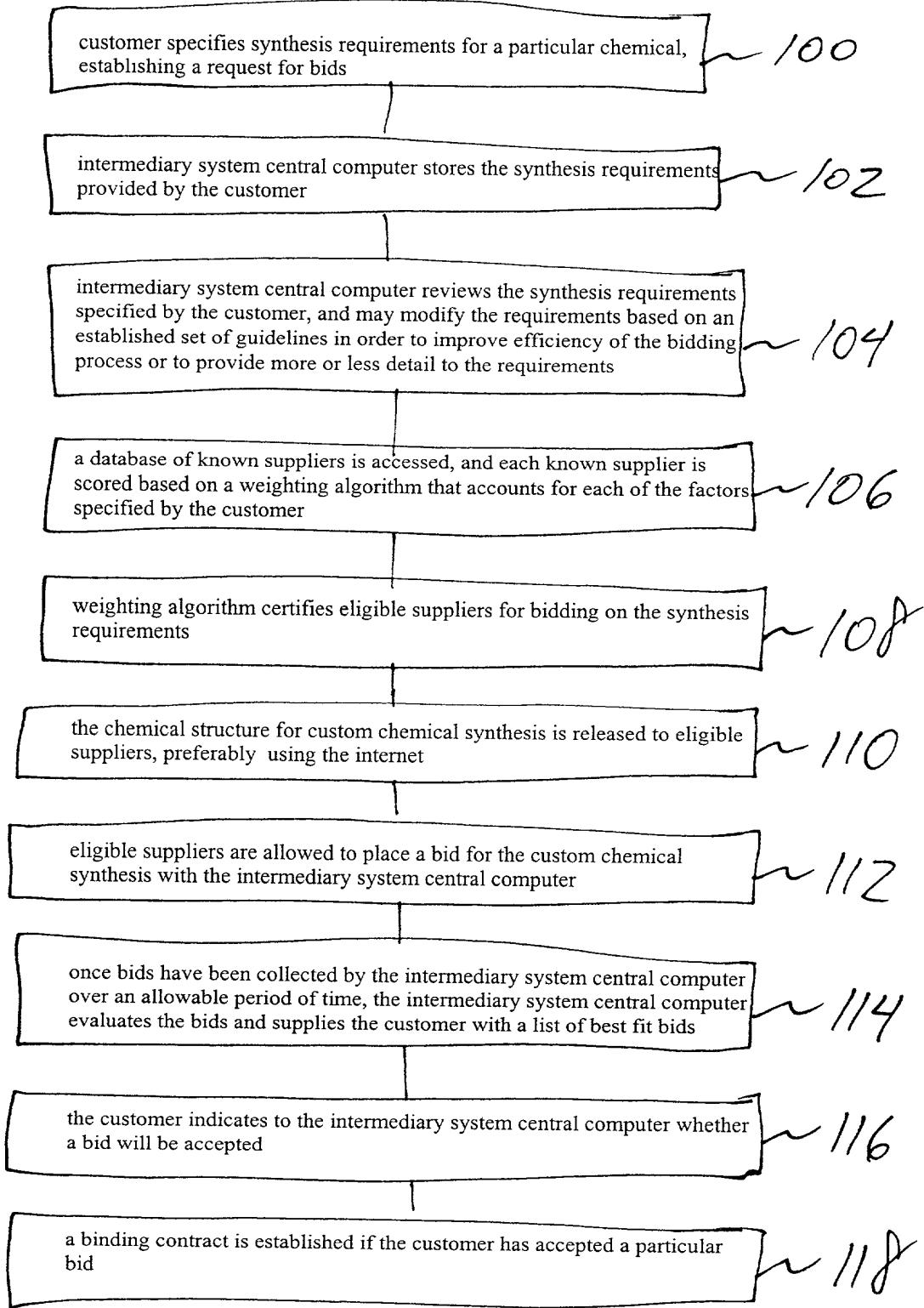


Fig. 3

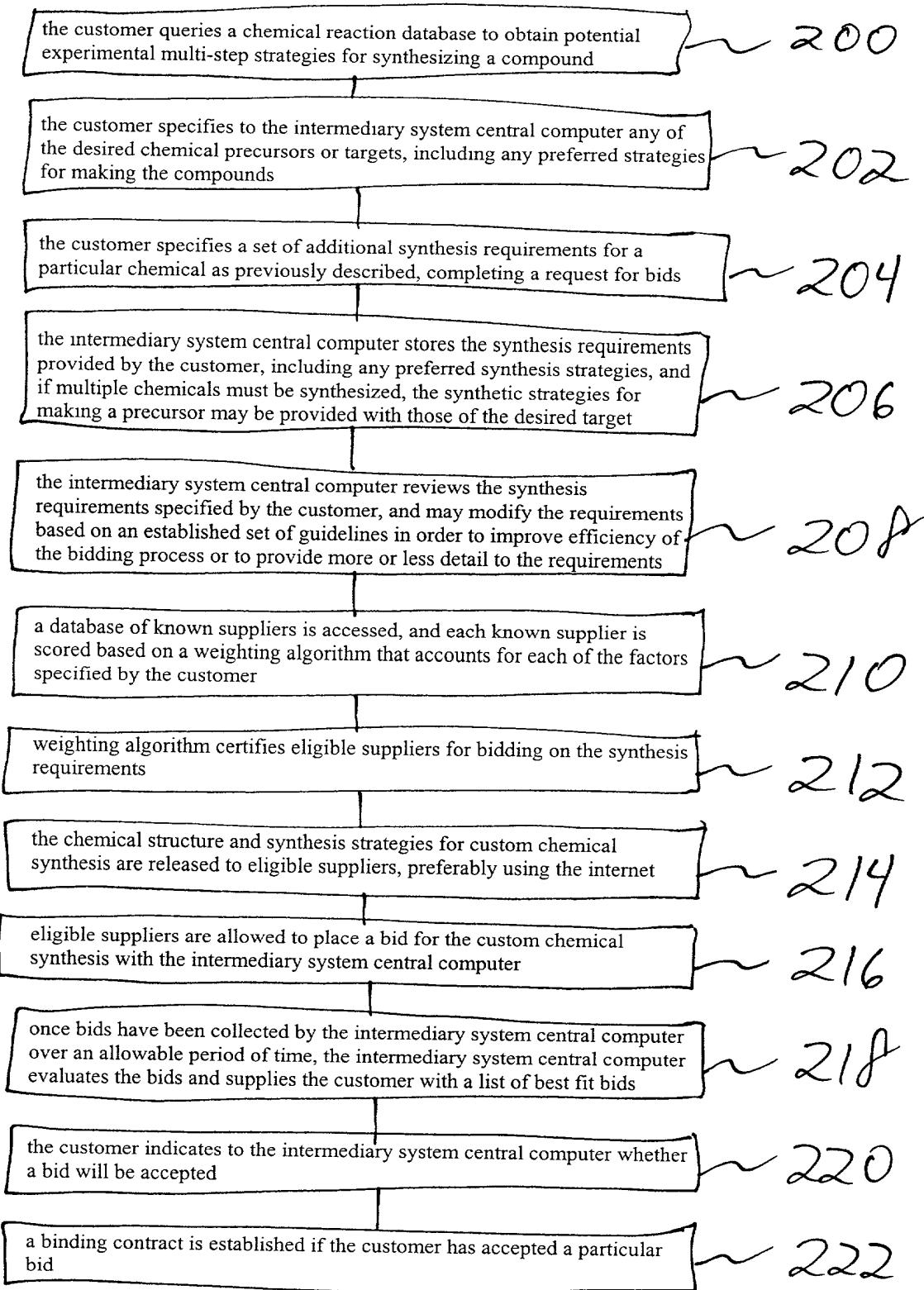


Fig. 4

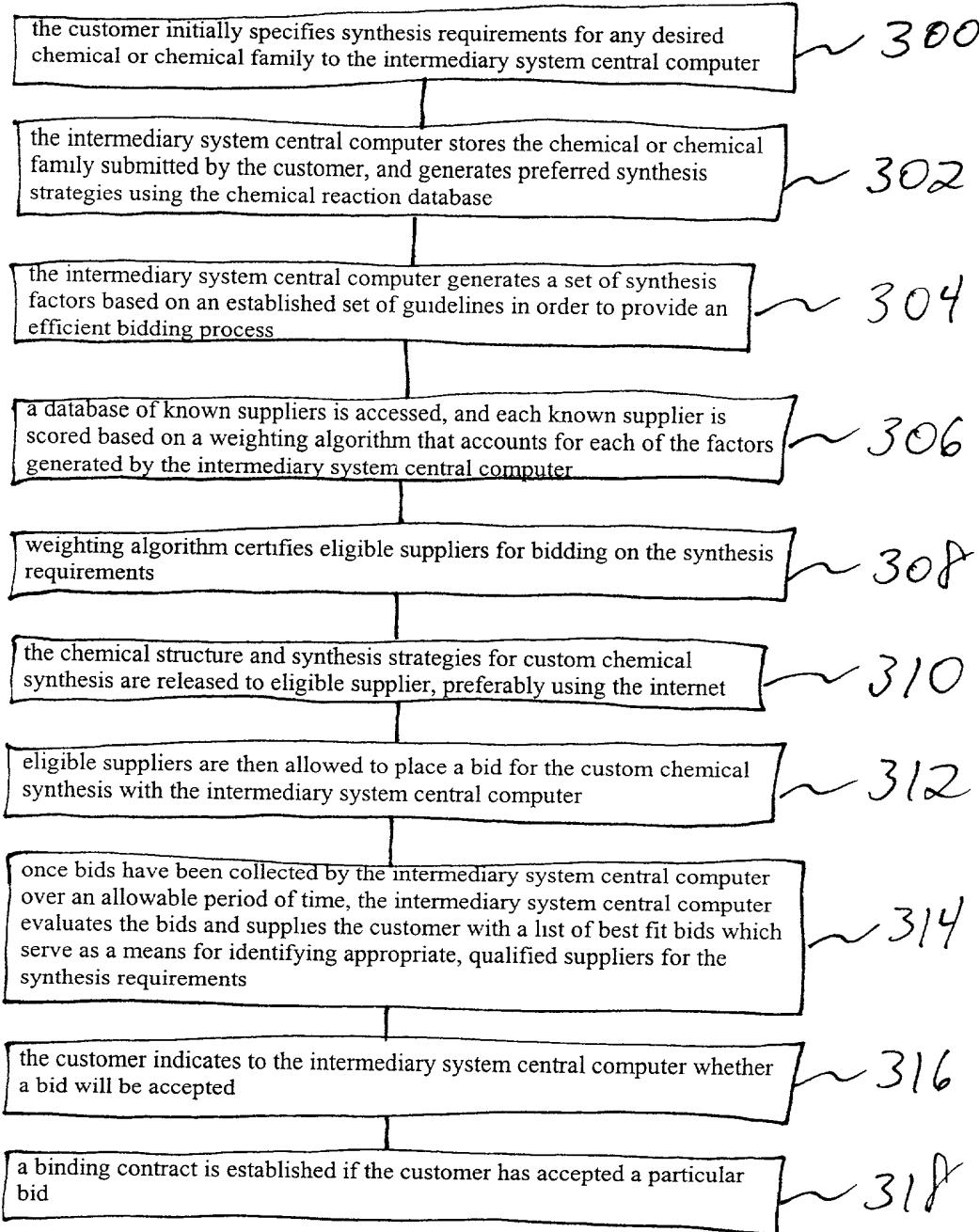


Fig. 5

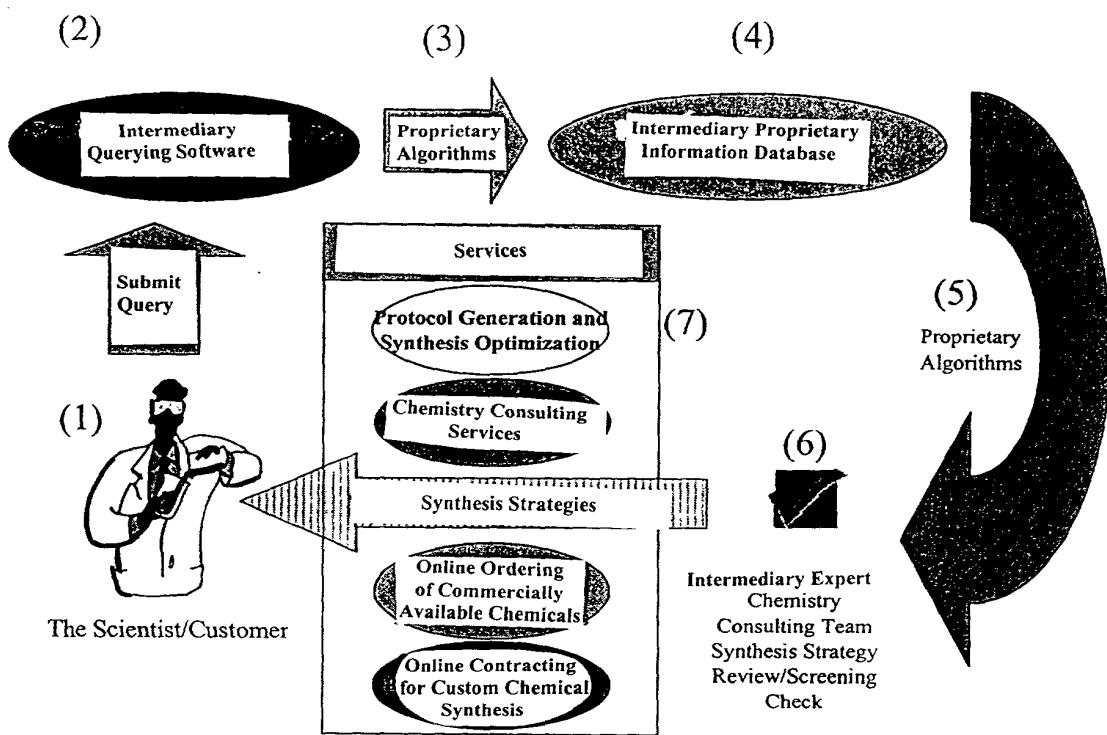
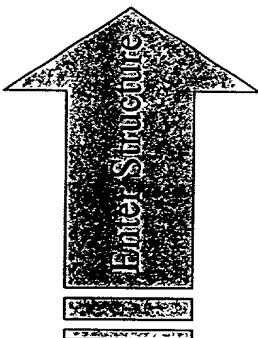
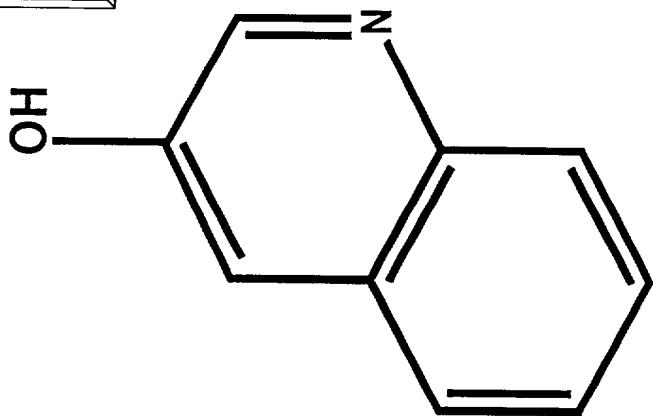


Fig. 6



## Target Structure Entry

Analyze



400

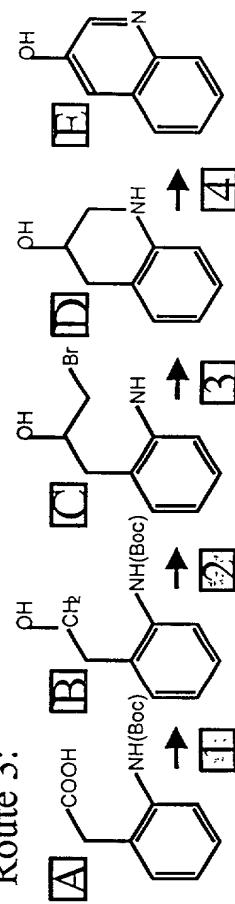
Fig. 7

# Synthesis Strategies

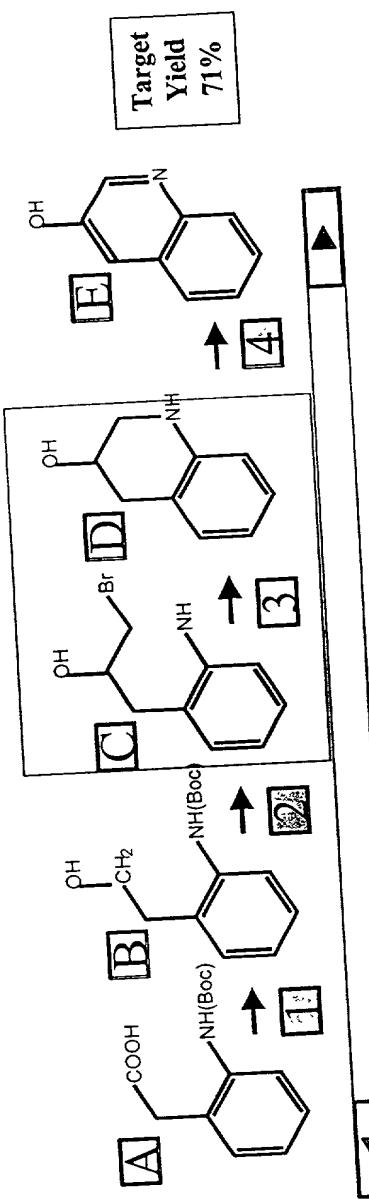
| Routes         | Yield %   | # of steps to ACD | # of Purification Steps Required | Cost Per mg of product | Add Synthetic Routes to Project |
|----------------|-----------|-------------------|----------------------------------|------------------------|---------------------------------|
| Route 1        | 86        | 6                 | 4                                | \$2,000                | ☒                               |
| Route 2        | 75        | N/A               | N/A                              | N/A                    | ☒                               |
| <b>Route 3</b> | <b>71</b> | <b>4</b>          | <b>3</b>                         | <b>\$6,434</b>         | <b>☒</b>                        |
| Route 4        | 63        | 5                 | 2                                | \$200                  | ☒                               |
| Route 5        | 44        | 10                | 8                                | \$22,050               | ☒                               |
| Route 6        | 31        | 7                 | 6                                | \$15,427               | ☒                               |
| Route 7        | 24        | 5                 | 5                                | \$155                  | ☒                               |
| Route 8        | 20        | 6                 | 4                                | \$4,450                | ☒                               |
| Route 9        | 17        | 6                 | 5                                | \$344                  | ☒                               |
| Route 10       | 9         | N/A               | N/A                              | N/A                    | ☒                               |
| Route 11       | 4         | 6                 | 6                                | \$36,000               | ☒                               |

420

Tig. J



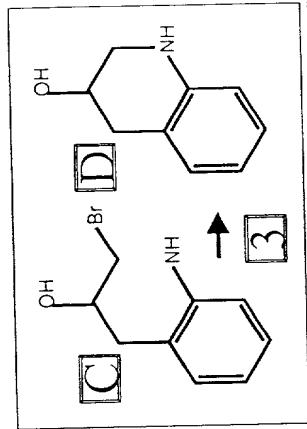
# Synthesis Reaction Planner



440

Fig. 9

# Synthesis Protocol Generation



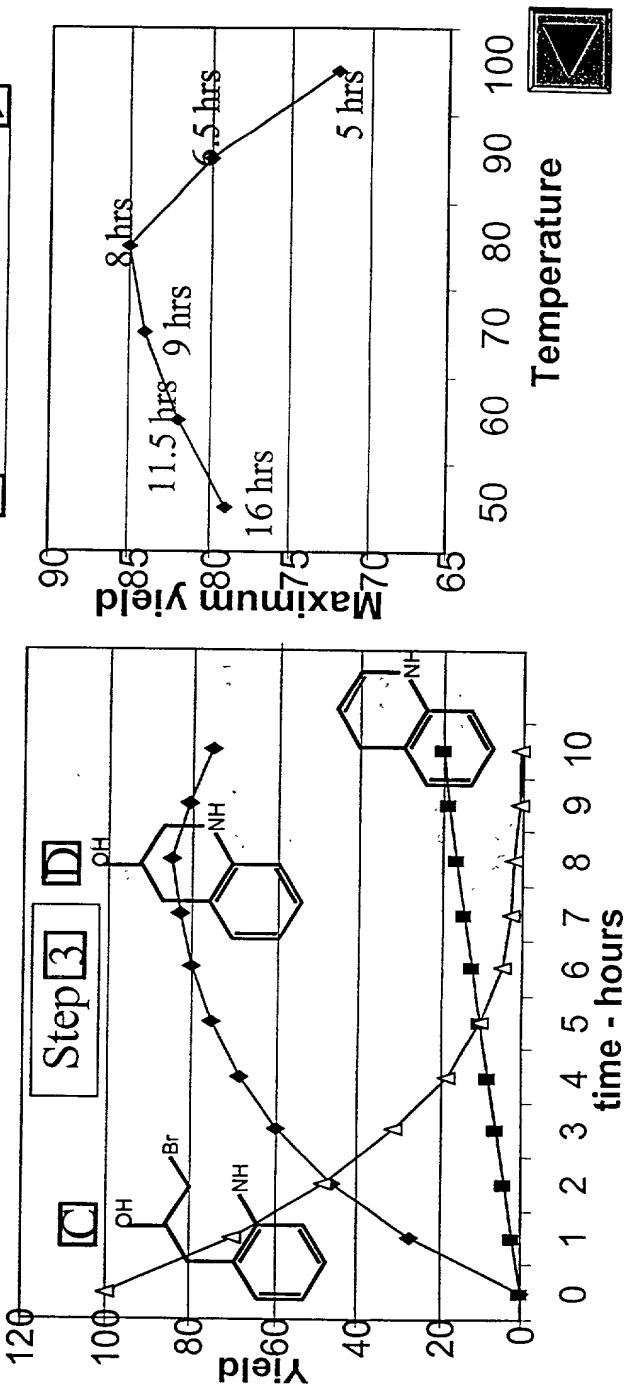
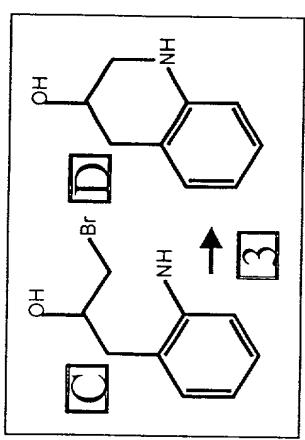
| Step | Starting materials in order of addition | Amount (g) | Inventory ID and Location | Solvent | Amount (ml) | Recommended purification steps              | Time | Temp. | Scheduled date for completion     |
|------|---|------------|---------------------------|---------|-------------|---|------|-------|-----------------------------------|
|      |   |            |                           |         |             | <input type="checkbox"/> View Side Products |      |       |                                   |
| 3    |   |            |                           |         |             |   |      |       | <input type="checkbox"/> Optimize |

460

Fig. 10

# Synthesis Reaction Optimization

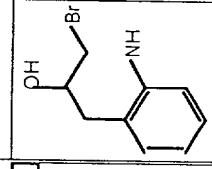
| Optimize the Reaction Time and Temperature for Step <b>3</b> |            |
|--|------------|
| Temperature 80° C  | Time 8 Hrs |



480

Fig. 11

# Request Bids

| Target   | Level of Confidentiality Required      | Desired Quantity | Cost       | Level of Purity         | Stereo-chemical Requirements | Suggested Strategies          | Request Bids                                  |
|--|--|------------------|------------|-------------------------|------------------------------|-------------------------------|---|
|  |  |                  |            |                         |                              |                               | Request Preliminary Bids                      |
| <br><input type="checkbox"/> <input checked="" type="checkbox"/> <input type="checkbox"/> | Ultra<br>High<br>Medium<br>Low<br>None | 10 g             | < \$40,000 | ✓ 99%<br>✓ 95%<br>✓ 90% | None                         | <input type="checkbox"/> Edit | <input type="checkbox"/> Request Binding Bids |

500

Fig. 12